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Study of neutral Fe(III) complexes of pyridoxal-N-substituted thiosemicarbazone with desolvation-induced spin-state transformation above room temperature

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```

# CIF-file generated for C19H31FeN8O8S2          P-1          q1115
#=====
data_DATNAM
#=====

# 0. AUDIT DETAILS

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_audit_creation_method
;
  PLATON <TABLE ACC> option    (version ::  40506)
  SHELXL97-2 & Manual Editing
;
_audit_update_record
;
?
;

#=====

# 1. SUBMISSION DETAILS

_publ_contact_author_name      # Name   of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address    # Address of author for correspondence
;
  Crystal Structure Center,
  Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen,
  The Netherlands.
;
_publ_contact_author_email      A.Meetsma@rug.nl
_publ_contact_author_fax        '+31 50 3634441'
_publ_contact_author_phone      '+31 50 3634368'

_publ_requested_journal         'Inorganic Chemistry'
# Publication choise FI, CI or EI for Inorganic
#                               FM, CM or EM for Metal-organic
#                               FO, CO or EO for Organic
_publ_requested_category        ?
_publ_requested_coeditor_name   ?

_publ_contact_letter            # Include date of submission
;
  Date of submission :  2006-08-20  14:04:48

  Consider this CIF submission for deposition of the second
  X-ray structure of a manuscript to be submitted to : Inorganic Chemistry
  (Our Compound_Identification_Code : Q1115)
;

#=====

# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic   ?

```

```

_journal_date_to_coeditor      ?
_journal_date_from_coeditor    ?
_journal_date_accepted         ?

_journal_date_printers_first   ?
_journal_date_printers_final   ?
_journal_date_proofs_out       ?
_journal_date_proofs_in        ?

_journal_coeditor_name         ?
_journal_coeditor_code         ?
_journal_coeditor_notes
;
;

_journal_techeditor_code       ?
_journal_techeditor_notes
;
;

_journal_coden_ASTM            ?
_journal_name_full             ?
_journal_year                  ?
_journal_volume                ?
_journal_issue                 ?
_journal_page_first            ?
_journal_page_last             ?

_journal_suppl_publ_number     ?
_journal_suppl_publ_pages      ?

```

```
#=====
```

3. TITLE AND AUTHOR LIST

```

_publ_section_title
;
?
;
_publ_section_title_footnote
;
?
;

```

```

# The loop structure below should contain the names and addresses of all
# authors, in the required order of publication. Repeat as necessary.

```

```

loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
; # author related footnote
;
; # Address of this author
;
'Meetsma, Auke'

```

```

;
? # author related footnote
;
;
    Crystal Structure Center,
    Chemical Physics,
    Zernike Institute for Advanced Materials
    University of Groningen,
    Nijenborgh 4,
    NL-9747 AG Groningen,
    The Netherlands.
;

#=====

# 4. TEXT

_publ_section_synopsis
;
?
;
_publ_section_abstract
;
?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
    The asymmetric unit consists of five moieties: a Fe-complex,
    an highly disordered methanol solvate molecule and three water solvate
    molecules.
;
_publ_section_exptl_prep
;
?
;
_publ_section_exptl_refinement
;
    The structure was solved by direct methods using the program SIR2002.
    The positional and anisotropic displacement parameters for the non-hydrogen
    atoms were refined. A subsequent difference Fourier synthesis resulted in
    the location of the hydrogen atoms of the Fe-complex, which coordinates
    and isotropic displacement parameters were refined.
    Refinement was frustrated by a disorder problem: from the solution,
    it was clear that the atom positions of the solvate molecules were
    highly disordered: suggesting dynamic disorder (dynamic means that
    the smeared electron density is due to fluctuations of the atomic positions
    within each unit cell) as a consequence of translational- and rotational-
    disorder);
    the disorder is compensated by the larger the displacement parameters).
    The electron density for methanol solvate molecule has been described by
    two sites: each with an s.o.f of 0.5.
    The hydrogen atoms of the solvate molecules were generated by geometrical
    considerations, constrained to idealized geometries, and allowed to ride
    on their carrier atoms with an isotropic displacement parameter related to
    the equivalent displacement parameter of their carrier atoms.
    To improve the hydrogen parameters chemical more reasonable, ultimately
    restrain instructions (DFIX, DANG), were applied in the refinement
;

```

Insert blank lines between references

_publ_section_references

;

Allen, F.H. (2000). Acta Cryst. B58, 380-388.

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University of Groningen, The Netherlands. (unpublished).

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Multi-Scan Absorption Correction Program.

University of Göttingen, Germany.

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Wilson, A.J.C. (1992). Ed. International Tables for Crystallography,

Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.

;

_publ_section_figure_captions

;

Fig. 1. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound.

Displacement ellipsoids for non-H are represented at the 50% probability level.

The H-atoms have been omitted to improve clarity.

;

#=====

5. CHEMICAL DATA

```
_chemical_name_systematic
;
;
_chemical_name_common          ?
_chemical_melting_point        ?
_chemical_formula_moiety
'C18 H21 Fe N8 O4 S2, 0.5(C2 H8 O2), 3(H2 O) '
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O) '
_chemical_formula_structural   ?
_chemical_formula_sum
'C19 H31 Fe N8 O8 S2'
_chemical_formula_iupac        ?
_chemical_formula_weight       619.48
_chemical_compound_source      'see text'
```

```
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
S   S   0.1246   0.1234
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O   O   0.0106   0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N   N   0.0061   0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe  Fe   0.3463   0.8444
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H   H   0.0000   0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C   C   0.0033   0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
```

#=====

6. CRYSTAL DATA

```
_symmetry_cell_setting          Triclinic
_symmetry_space_group_name_Hall '-P 1'
_symmetry_space_group_name_H-M  'P -1'
_symmetry_Int_Tables_number     2
```

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
```

```
_cell_length_a      10.701(2)
_cell_length_b      10.846(2)
_cell_length_c      11.910(2)
_cell_angle_alpha    83.347(3)
_cell_angle_beta     83.896(3)
_cell_angle_gamma    68.914(3)
_cell_volume         1278.0(4)
```

```

_cell_formula_units_Z          2
_cell_measurement_temperature  100(1)
_cell_measurement_reflns_used   2956
_cell_measurement_theta_min     2.54
_cell_measurement_theta_max     28.53
_cell_special_details

```

```

;
  The final unit cell was obtained from the xyz centroids of
  2956 reflections after integration using the SAINTPLUS
  software package (Bruker, 2000).

```

```

  The unit cell was identified as triclinic, space group, P-1,
  although reduced cell calculations indicate (pseudo) metric monoclinic
  C-centered lattice symmetry4, but examination of the final atomic
  coordinates of the structure did not support for the extra metric
  symmetry elements (Spek, 1988; Le Page 1987, 1988).

```

```

;

```

```

_exptl_crystal_description      'platelet'
_exptl_crystal_colour           'green'
_exptl_crystal_size_max         0.27
_exptl_crystal_size_mid         0.23
_exptl_crystal_size_min         0.07
_exptl_crystal_size_rad         ?
_exptl_crystal_density_meas     ?
_exptl_crystal_density_diffn    1.610
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000            646
_exptl_absorpt_coefficient_mu    0.815
_exptl_absorpt_correction_type   'Multi-Scan'
_exptl_absorpt_process_details   '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min  0.8342
_exptl_absorpt_correction_T_max  0.9452

```

```

#=====

```

``` # 7. EXPERIMENTAL DATA ```

```

_exptl_special_details
;
;
_diffn_ambient_temperature      100(1)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           'MoK\alpha'
_diffn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator   'parallel mounted graphite'
_diffn_radiation_detector
;
  CCD area-detector
;
_diffn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
_diffn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean  '4096x4096 / 62x62 (binned 512)'

```

```
_diffrn_standards_number      0
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%      0
```

```
loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?
```

```
# number of measured reflections (redundant set)
```

```
_diffrn_reflns_number      9700
_diffrn_reflns_av_R_equivalents  0.0412
_diffrn_reflns_av_sigmaI/netI  0.0748
_diffrn_reflns_limit_h_min   -13
_diffrn_reflns_limit_h_max    12
_diffrn_reflns_limit_k_min   -13
_diffrn_reflns_limit_k_max    12
_diffrn_reflns_limit_l_min   -14
_diffrn_reflns_limit_l_max    14
_diffrn_reflns_theta_min     2.58
_diffrn_reflns_theta_max    26.01
_diffrn_measured_fraction_theta_max  0.971
_diffrn_reflns_theta_full    25.00
_diffrn_measured_fraction_theta_full  0.980
```

```
_diffrn_reflns_reduction_process
```

```
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;
```

```
# number of unique reflections
```

```
_reflns_number_total      4874
_reflns_number_gt         3702
_reflns_threshold_expression  I>2\sigma(I)
```

```
_computing_data_collection  'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement  'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction   'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
```

```
;
SIR2002 (Burla et al., 2003)
```

```
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
```

```
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
```

```
;
_computing_publication_material  'PLATON (Spek, 2003)'
```

```
#=====
```

```
# 8. REFINEMENT DATA
```



```
_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;
```

```
_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\s2(Fo2)+(0.0588P)2+3.20P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment mixed
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?
```

```
_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 4874
_refine_ls_number_parameters 469
_refine_ls_number_restraints 9
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0801
_refine_ls_R_factor_gt 0.0560
_refine_ls_wR_factor_ref 0.1424
_refine_ls_wR_factor_gt 0.1301
_refine_ls_goodness_of_fit_ref 1.041
_refine_ls_restrained_S_all 1.042
_refine_ls_shift/su_max 1.169
_refine_ls_shift/su_mean 0.018
```

```
_refine_diff_density_max 1.612
_refine_diff_density_min -0.943
_refine_diff_density_rms 0.112
```

```
_vrn_publ_code_frame_time_sec 20.0
_vrn_publ_code_meas_time_hour 13.5
```

```
#=====
```

``` # 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS ```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
```

Fe	Fe	Uani	0.33148(6)	0.87790(6)	0.31984(5)	1.000	0.0106(2)	. . .
S1	S	Uani	0.13051(10)	0.89042(10)	0.40686(9)	1.000	0.0144(3)	. . .
S2	S	Uani	0.29420(11)	1.08272(10)	0.37074(8)	1.000	0.0139(3)	. . .
O1	O	Uani	0.5036(3)	0.8603(3)	0.2395(2)	1.000	0.0126(8)	. . .
O2	O	Uani	0.2769(3)	0.8223(3)	-0.1354(3)	1.000	0.0190(10)	. . .
O3	O	Uani	0.3629(3)	0.6991(3)	0.2856(2)	1.000	0.0153(9)	. . .
O4	O	Uani	0.8222(3)	0.5841(3)	0.4844(3)	1.000	0.0185(10)	. . .
N1	N	Uani	0.2344(3)	0.9463(3)	0.1865(3)	1.000	0.0124(10)	. . .
N2	N	Uani	0.6963(4)	0.7508(3)	-0.0172(3)	1.000	0.0150(11)	. . .
N3	N	Uani	0.0953(3)	1.0148(3)	0.1955(3)	1.000	0.0149(11)	. . .
N4	N	Uani	-0.0932(4)	1.0411(4)	0.3114(4)	1.000	0.0203(12)	. . .
N5	N	Uani	0.4209(3)	0.8181(3)	0.4576(3)	1.000	0.0111(10)	. . .
N6	N	Uani	0.6366(4)	0.3919(3)	0.2577(3)	1.000	0.0185(11)	. . .
N7	N	Uani	0.3939(3)	0.9013(3)	0.5455(3)	1.000	0.0128(10)	. . .
N8	N	Uani	0.3125(4)	1.1186(4)	0.5849(3)	1.000	0.0143(11)	. . .
C1	C	Uani	0.2873(4)	0.9407(4)	0.0830(3)	1.000	0.0127(12)	. . .
C2	C	Uani	0.4288(4)	0.8752(4)	0.0522(3)	1.000	0.0114(11)	. . .
C3	C	Uani	0.4692(4)	0.8532(4)	-0.0628(3)	1.000	0.0136(11)	. . .
C4	C	Uani	0.6025(4)	0.7931(4)	-0.0930(4)	1.000	0.0167(12)	. . .
C5	C	Uani	0.6639(4)	0.7703(4)	0.0932(3)	1.000	0.0128(11)	. . .
C6	C	Uani	0.5274(4)	0.8378(4)	0.1318(3)	1.000	0.0126(11)	. . .
C7	C	Uani	0.3700(5)	0.8922(4)	-0.1534(3)	1.000	0.0170(12)	. . .
C8	C	Uani	0.7726(5)	0.7153(5)	0.1722(4)	1.000	0.0174(12)	. . .
C9	C	Uani	0.0408(4)	0.9881(4)	0.2967(3)	1.000	0.0147(12)	. . .
C10	C	Uani	0.5094(4)	0.7014(4)	0.4794(3)	1.000	0.0125(12)	. . .
C11	C	Uani	0.5528(4)	0.5986(4)	0.4002(3)	1.000	0.0138(12)	. . .
C12	C	Uani	0.6732(4)	0.4897(4)	0.4158(3)	1.000	0.0143(12)	. . .
C13	C	Uani	0.7102(4)	0.3901(4)	0.3435(4)	1.000	0.0176(12)	. . .
C14	C	Uani	0.5237(4)	0.4937(4)	0.2410(3)	1.000	0.0165(12)	. . .
C15	C	Uani	0.4762(4)	0.6023(4)	0.3099(3)	1.000	0.0139(12)	. . .
C16	C	Uani	0.7652(4)	0.4814(4)	0.5059(4)	1.000	0.0161(12)	. . .
C17	C	Uani	0.4432(5)	0.4943(5)	0.1453(4)	1.000	0.0210(14)	. . .
C18	C	Uani	0.3384(4)	1.0267(4)	0.5087(3)	1.000	0.0141(12)	. . .
O8A	O	Uani	0.1572(11)	0.5508(9)	-0.0054(10)	0.500	0.071(4)	. . .
O8B	O	Uani	-0.0044(11)	0.8873(10)	0.0503(7)	0.500	0.053(3)	. . .
C81A	C	Uani	0.145(5)	0.681(10)	0.000(2)	0.500	0.45(6)	. . .
C81B	C	Uani	0.0599(19)	0.788(2)	-0.0156(16)	0.500	0.085(8)	. . .
O5	O	Uani	0.0342(4)	0.4763(4)	0.3194(3)	1.000	0.0286(11)	. . .
O6	O	Uani	0.1226(4)	0.6728(4)	0.2107(4)	1.000	0.0462(14)	. . .
O7	O	Uani	0.0529(5)	0.3032(5)	0.1432(4)	1.000	0.0619(17)	. . .
H1	H	Uiso	0.229(4)	0.981(4)	0.025(4)	1.000	0.011(11)	. . .
H4	H	Uiso	0.636(5)	0.779(5)	-0.166(4)	1.000	0.028(14)	. . .
H7	H	Uiso	0.426(4)	0.872(4)	-0.229(4)	1.000	0.014(11)	. . .
H7'	H	Uiso	0.319(4)	0.989(5)	-0.162(4)	1.000	0.016(12)	. . .
H8	H	Uiso	0.752(5)	0.665(5)	0.238(5)	1.000	0.034(15)	. . .
H8'	H	Uiso	0.849(5)	0.668(5)	0.134(4)	1.000	0.020(12)	. . .
H8''	H	Uiso	0.797(6)	0.773(6)	0.193(5)	1.000	0.042(18)	. . .
H10	H	Uiso	0.552(4)	0.678(4)	0.556(3)	1.000	0.010(10)	. . .
H13	H	Uiso	0.787(5)	0.317(5)	0.353(4)	1.000	0.019(12)	. . .
H16	H	Uiso	0.838(4)	0.390(4)	0.514(4)	1.000	0.012(11)	. . .
H16'	H	Uiso	0.717(4)	0.493(4)	0.583(4)	1.000	0.011(11)	. . .
H17	H	Uiso	0.353(4)	0.481(4)	0.173(4)	1.000	0.011(11)	. . .
H17'	H	Uiso	0.409(4)	0.577(5)	0.104(4)	1.000	0.014(11)	. . .
H17''	H	Uiso	0.500(5)	0.432(5)	0.100(4)	1.000	0.034(15)	. . .
H22	H	Uiso	0.308(5)	0.756(6)	-0.166(5)	1.000	0.032(16)	. . .
H24	H	Uiso	0.886(9)	0.580(9)	0.436(8)	1.000	0.12(4)	. . .
H25	H	Uiso	0.774(11)	0.731(11)	-0.045(10)	1.000	0.17(5)	. . .
H26	H	Uiso	-0.135(5)	1.080(5)	0.252(5)	1.000	0.022(14)	. . .
H26'	H	Uiso	-0.119(5)	1.025(5)	0.367(4)	1.000	0.013(13)	. . .
H27	H	Uiso	0.284(5)	1.193(5)	0.557(4)	1.000	0.017(13)	. . .
H27'	H	Uiso	0.364(5)	1.090(5)	0.642(4)	1.000	0.024(14)	. . .

H811' H Uiso 0.05365 0.73954 -0.01622 0.500 0.6707 . .
 H811" H Uiso 0.20959 0.70328 -0.05529 0.500 0.6707 . .
 H812' H Uiso -0.00305 0.74701 -0.03312 0.500 0.1247 . .
 H812" H Uiso 0.13359 0.72141 0.02440 0.500 0.1247 . .
 H81 H Uiso 0.09372 0.54843 -0.03996 0.500 0.1056 . .
 H82 H Uiso -0.07426 0.87699 0.08210 0.500 0.0789 . .
 H811 H Uiso 0.16279 0.69322 0.07656 0.500 0.6707 . .
 H812 H Uiso 0.09602 0.82274 -0.08610 0.500 0.1247 . .
 H51 H Uiso 0.061(7) 0.534(6) 0.279(6) 1.000 0.09(3) . .
 H51' H Uiso 0.103(6) 0.431(9) 0.357(8) 1.000 0.17(5) . .
 H61 H Uiso 0.193(4) 0.685(6) 0.226(5) 1.000 0.05(2) . .
 H61' H Uiso 0.089(6) 0.736(5) 0.160(5) 1.000 0.09(3) . .
 H71 H Uiso 0.033(8) 0.376(4) 0.093(4) 1.000 0.0741 . .
 H71' H Uiso 0.037(7) 0.341(5) 0.206(3) 1.000 0.0741 . .

loop_

_atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12

Fe 0.0141(3) 0.0089(3) 0.0100(3) -0.0062(2) 0.0002(2) -0.0041(2)
 S1 0.0158(5) 0.0144(5) 0.0132(5) -0.0053(4) 0.0007(4) -0.0048(4)
 S2 0.0211(5) 0.0103(5) 0.0118(5) -0.0061(4) -0.0017(4) -0.0058(4)
 O1 0.0153(15) 0.0135(14) 0.0094(14) -0.0050(11) -0.0001(11) -0.0044(12)
 O2 0.0239(17) 0.0150(16) 0.0210(17) -0.0077(14) -0.0057(13) -0.0075(14)
 O3 0.0168(15) 0.0161(15) 0.0143(15) -0.0090(12) -0.0006(12) -0.0053(12)
 O4 0.0216(17) 0.0161(16) 0.0213(17) -0.0046(13) -0.0032(14) -0.0096(13)
 N1 0.0181(18) 0.0072(16) 0.0144(18) -0.0083(14) 0.0015(14) -0.0059(14)
 N2 0.020(2) 0.0147(18) 0.0109(18) -0.0067(14) 0.0027(14) -0.0063(15)
 N3 0.0125(18) 0.0131(18) 0.0188(19) -0.0066(15) -0.0022(14) -0.0024(14)
 N4 0.020(2) 0.026(2) 0.013(2) -0.0042(18) 0.0000(18) -0.0055(17)
 N5 0.0123(17) 0.0123(17) 0.0124(17) -0.0075(14) 0.0043(13) -0.0082(14)
 N6 0.022(2) 0.0129(18) 0.023(2) -0.0073(15) -0.0005(16) -0.0075(15)
 N7 0.0184(18) 0.0115(17) 0.0100(17) -0.0088(14) 0.0001(14) -0.0051(14)
 N8 0.021(2) 0.0087(19) 0.0127(19) -0.0045(15) -0.0027(15) -0.0033(16)
 C1 0.020(2) 0.009(2) 0.011(2) -0.0026(16) -0.0032(17) -0.0063(17)
 C2 0.016(2) 0.0096(19) 0.0090(19) -0.0029(15) -0.0012(16) -0.0041(16)
 C3 0.026(2) 0.0079(19) 0.010(2) -0.0022(16) -0.0021(17) -0.0091(17)
 C4 0.026(2) 0.016(2) 0.011(2) -0.0075(17) 0.0016(18) -0.0098(19)
 C5 0.022(2) 0.0060(19) 0.011(2) -0.0037(15) 0.0012(16) -0.0053(16)
 C6 0.022(2) 0.0049(19) 0.014(2) -0.0049(15) 0.0010(17) -0.0077(16)
 C7 0.028(2) 0.015(2) 0.010(2) -0.0017(17) -0.0029(18) -0.0092(19)
 C8 0.019(2) 0.017(2) 0.016(2) -0.0059(19) 0.0003(18) -0.005(2)
 C9 0.017(2) 0.012(2) 0.017(2) -0.0086(17) 0.0004(17) -0.0057(17)
 C10 0.014(2) 0.013(2) 0.013(2) -0.0025(16) -0.0025(16) -0.0069(17)
 C11 0.017(2) 0.012(2) 0.015(2) -0.0060(16) 0.0023(16) -0.0077(17)
 C12 0.018(2) 0.014(2) 0.013(2) -0.0016(16) 0.0009(16) -0.0085(17)
 C13 0.018(2) 0.009(2) 0.023(2) -0.0065(18) -0.0010(18) 0.0001(18)
 C14 0.024(2) 0.015(2) 0.013(2) -0.0068(17) 0.0035(17) -0.0094(18)
 C15 0.021(2) 0.008(2) 0.015(2) -0.0043(16) 0.0008(17) -0.0073(17)
 C16 0.019(2) 0.010(2) 0.020(2) -0.0007(17) -0.0029(18) -0.0057(17)
 C17 0.026(3) 0.017(2) 0.020(2) -0.010(2) -0.005(2) -0.004(2)
 C18 0.014(2) 0.020(2) 0.011(2) -0.0081(17) 0.0030(16) -0.0084(17)

 O8A 0.061(7) 0.040(5) 0.105(9) -0.045(6) -0.057(6) 0.015(5)
 O8B 0.082(7) 0.071(6) 0.032(5) -0.005(4) -0.010(5) -0.058(6)
 C81A 0.26(5) 1.24(18) 0.059(16) 0.10(5) -0.07(3) -0.55(9)
 C81B 0.061(11) 0.18(2) 0.051(11) -0.016(12) 0.009(9) -0.090(13)

```

O5 0.032(2) 0.032(2) 0.0263(19) -0.0071(16) -0.0035(16) -0.0147(17)
O6 0.040(2) 0.035(2) 0.072(3) -0.005(2) -0.015(2) -0.020(2)
O7 0.054(3) 0.078(3) 0.054(3) -0.037(3) 0.007(2) -0.017(3)

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``` # 10. MOLECULAR GEOMETRY ```

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_geom_special_details

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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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loop_

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_geom_bond_atom_site_label_1

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_geom_bond_atom_site_label_2

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_geom_bond_distance

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_geom_bond_site_symmetry_1

```

```

_geom_bond_site_symmetry_2

```

```

_geom_bond_publ_flag

```

Fe	S1	2.2508(14)	.	.	yes
Fe	S2	2.2549(13)	.	.	yes
Fe	O1	1.939(3)	.	.	yes
Fe	O3	1.930(3)	.	.	yes
Fe	N1	1.917(4)	.	.	yes
Fe	N5	1.916(4)	.	.	yes
S1	C9	1.726(4)	.	.	yes
S2	C18	1.738(4)	.	.	yes
O1	C6	1.315(4)	.	.	yes
O2	C7	1.440(6)	.	.	yes
O3	C15	1.321(5)	.	.	yes
O4	C16	1.438(5)	.	.	yes
O2	H22	0.79(6)	.	.	no
O4	H24	0.84(10)	.	.	no
O8A	C81A	1.38(10)	.	.	yes
O8B	C81B	1.34(2)	.	.	yes
O8A	H81	0.8400	.	.	no
O8B	H82	0.8400	.	.	no
O5	H51'	0.86(9)	.	.	no
O5	H51	0.86(7)	.	.	no
O6	H61	0.85(5)	.	.	no
O6	H61'	0.86(5)	.	.	no
O7	H71'	0.87(4)	.	.	no
O7	H71	0.91(4)	.	.	no
N1	N3	1.403(5)	.	.	yes
N1	C1	1.299(5)	.	.	yes
N2	C4	1.341(6)	.	.	yes
N2	C5	1.345(5)	.	.	yes
N3	C9	1.330(5)	.	.	yes
N4	C9	1.339(6)	.	.	yes
N5	C10	1.296(5)	.	.	yes
N5	N7	1.400(5)	.	.	yes
N6	C13	1.349(6)	.	.	yes
N6	C14	1.326(6)	.	.	yes
N7	C18	1.316(5)	.	.	yes
N8	C18	1.361(5)	.	.	yes

N2	H25	0.82 (12)	.	.	no
N4	H26	0.86 (6)	.	.	no
N4	H26'	0.72 (5)	.	.	no
N8	H27	0.80 (5)	.	.	no
N8	H27'	0.88 (5)	.	.	no
C1	C2	1.449 (6)	.	.	no
C2	C3	1.413 (5)	.	.	no
C2	C6	1.412 (6)	.	.	no
C3	C7	1.512 (6)	.	.	no
C3	C4	1.366 (6)	.	.	no
C5	C8	1.482 (7)	.	.	no
C5	C6	1.431 (6)	.	.	no
C10	C11	1.458 (5)	.	.	no
C11	C15	1.409 (6)	.	.	no
C11	C12	1.412 (6)	.	.	no
C12	C16	1.506 (6)	.	.	no
C12	C13	1.379 (6)	.	.	no
C14	C15	1.423 (6)	.	.	no
C14	C17	1.498 (7)	.	.	no
C1	H1	0.94 (5)	.	.	no
C4	H4	0.91 (5)	.	.	no
C7	H7	1.03 (5)	.	.	no
C7	H7'	0.99 (5)	.	.	no
C8	H8'	0.90 (5)	.	.	no
C8	H8"	0.83 (7)	.	.	no
C8	H8	0.96 (6)	.	.	no
C10	H10	1.03 (4)	.	.	no
C13	H13	0.92 (5)	.	.	no
C16	H16'	1.00 (5)	.	.	no
C16	H16	1.02 (4)	.	.	no
C17	H17"	0.92 (5)	.	.	no
C17	H17	1.04 (5)	.	.	no
C17	H17'	0.94 (5)	.	.	no
C81A	C81B	1.20 (10)	.	.	no
C81A	H811'	0.9800	.	.	no
C81A	H811	0.9800	.	.	no
C81A	H811"	0.9800	.	.	no
C81A	H812"	0.5200	.	.	no
C81B	H812	0.9800	.	.	no
C81B	H811'	0.5500	.	.	no
C81B	H812'	0.9800	.	.	no
C81B	H812"	0.9800	.	.	no
loop_					
_geom_angle_atom_site_label_1					
_geom_angle_atom_site_label_2					
_geom_angle_atom_site_label_3					
_geom_angle					
_geom_angle_site_symmetry_1					
_geom_angle_site_symmetry_2					
_geom_angle_site_symmetry_3					
_geom_angle_publ_flag					
S1	Fe	S2	88.38 (5)	.	yes
S1	Fe	O1	176.83 (10)	.	yes
S1	Fe	O3	90.02 (10)	.	yes
S1	Fe	N1	84.99 (11)	.	yes
S1	Fe	N5	92.91 (11)	.	yes
S2	Fe	O1	94.46 (10)	.	yes
S2	Fe	O3	176.64 (8)	.	yes
S2	Fe	N1	92.56 (10)	.	yes
S2	Fe	N5	84.70 (10)	.	yes

O1	Fe	O3	87.22 (13)	.	.	.	yes
O1	Fe	N1	93.47 (13)	.	.	.	yes
O1	Fe	N5	88.76 (13)	.	.	.	yes
O3	Fe	N1	90.25 (13)	.	.	.	yes
O3	Fe	N5	92.43 (12)	.	.	.	yes
N1	Fe	N5	176.60 (14)	.	.	.	yes
Fe	S1	C9	94.18 (15)	.	.	.	yes
Fe	S2	C18	93.86 (14)	.	.	.	yes
Fe	O1	C6	121.8 (3)	.	.	.	yes
Fe	O3	C15	120.5 (3)	.	.	.	yes
C7	O2	H22	109 (4)	.	.	.	no
C16	O4	H24	123 (6)	.	.	.	no
C81A	O8A	H81	109.00	.	.	.	no
C81B	O8B	H82	110.00	.	.	.	no
H51	O5	H51 '	103 (7)	.	.	.	no
H61	O6	H61 '	104 (6)	.	.	.	no
H71	O7	H71 '	100 (4)	.	.	.	no
Fe	N1	C1	125.4 (3)	.	.	.	yes
Fe	N1	N3	120.5 (3)	.	.	.	yes
N3	N1	C1	114.0 (3)	.	.	.	yes
C4	N2	C5	121.2 (4)	.	.	.	yes
N1	N3	C9	111.5 (3)	.	.	.	yes
Fe	N5	C10	125.1 (3)	.	.	.	yes
N7	N5	C10	113.9 (3)	.	.	.	yes
Fe	N5	N7	121.0 (2)	.	.	.	yes
C13	N6	C14	119.2 (3)	.	.	.	yes
N5	N7	C18	111.4 (3)	.	.	.	yes
C5	N2	H25	122 (9)	.	.	.	no
C4	N2	H25	115 (9)	.	.	.	no
H26	N4	H26 '	130 (6)	.	.	.	no
C9	N4	H26 '	113 (5)	.	.	.	no
C9	N4	H26	116 (4)	.	.	.	no
C18	N8	H27	113 (3)	.	.	.	no
H27	N8	H27 '	127 (5)	.	.	.	no
C18	N8	H27 '	113 (3)	.	.	.	no
N1	C1	C2	124.2 (4)	.	.	.	yes
C1	C2	C6	122.5 (3)	.	.	.	no
C3	C2	C6	119.2 (4)	.	.	.	no
C1	C2	C3	118.3 (4)	.	.	.	no
C4	C3	C7	118.8 (4)	.	.	.	no
C2	C3	C4	118.8 (4)	.	.	.	no
C2	C3	C7	122.4 (4)	.	.	.	no
N2	C4	C3	122.5 (4)	.	.	.	yes
C6	C5	C8	122.0 (3)	.	.	.	no
N2	C5	C8	117.8 (4)	.	.	.	yes
N2	C5	C6	120.1 (4)	.	.	.	yes
O1	C6	C2	125.0 (4)	.	.	.	yes
C2	C6	C5	118.0 (3)	.	.	.	no
O1	C6	C5	117.1 (4)	.	.	.	yes
O2	C7	C3	112.7 (3)	.	.	.	yes
S1	C9	N3	124.5 (3)	.	.	.	yes
N3	C9	N4	116.3 (4)	.	.	.	yes
S1	C9	N4	119.2 (3)	.	.	.	yes
N5	C10	C11	123.3 (4)	.	.	.	yes
C10	C11	C15	122.0 (4)	.	.	.	no
C12	C11	C15	118.6 (4)	.	.	.	no
C10	C11	C12	119.4 (4)	.	.	.	no
C11	C12	C16	122.2 (3)	.	.	.	no
C13	C12	C16	118.9 (4)	.	.	.	no
C11	C12	C13	118.9 (4)	.	.	.	no
N6	C13	C12	122.9 (4)	.	.	.	yes

N6	C14	C17	118.5 (4)	.	.	.	yes
C15	C14	C17	118.7 (4)	.	.	.	no
N6	C14	C15	122.8 (4)	.	.	.	yes
O3	C15	C14	117.9 (4)	.	.	.	yes
C11	C15	C14	117.6 (4)	.	.	.	no
O3	C15	C11	124.4 (4)	.	.	.	yes
O4	C16	C12	111.2 (4)	.	.	.	yes
N7	C18	N8	117.3 (3)	.	.	.	yes
S2	C18	N7	124.7 (3)	.	.	.	yes
S2	C18	N8	117.9 (3)	.	.	.	yes
N1	C1	H1	117 (3)	.	.	.	no
C2	C1	H1	119 (3)	.	.	.	no
C3	C4	H4	124 (3)	.	.	.	no
N2	C4	H4	114 (3)	.	.	.	no
C3	C7	H7	106 (3)	.	.	.	no
C3	C7	H7'	113 (3)	.	.	.	no
H7	C7	H7'	105 (4)	.	.	.	no
O2	C7	H7'	109 (3)	.	.	.	no
O2	C7	H7	111 (2)	.	.	.	no
H8'	C8	H8"	100 (6)	.	.	.	no
C5	C8	H8"	113 (4)	.	.	.	no
H8	C8	H8"	108 (5)	.	.	.	no
C5	C8	H8'	109 (3)	.	.	.	no
C5	C8	H8	115 (4)	.	.	.	no
H8	C8	H8'	112 (5)	.	.	.	no
N5	C10	H10	120 (2)	.	.	.	no
C11	C10	H10	117 (2)	.	.	.	no
N6	C13	H13	116 (3)	.	.	.	no
C12	C13	H13	121 (3)	.	.	.	no
C12	C16	H16	111 (3)	.	.	.	no
C12	C16	H16'	112 (3)	.	.	.	no
H16	C16	H16'	104 (4)	.	.	.	no
O4	C16	H16'	106 (2)	.	.	.	no
O4	C16	H16	111 (3)	.	.	.	no
H17'	C17	H17"	111 (4)	.	.	.	no
C14	C17	H17"	105 (3)	.	.	.	no
H17	C17	H17"	115 (4)	.	.	.	no
C14	C17	H17'	114 (3)	.	.	.	no
C14	C17	H17	113 (3)	.	.	.	no
H17	C17	H17'	99 (4)	.	.	.	no
O8A	C81A	C81B	137 (5)	.	.	.	yes
O8B	C81B	C81A	134 (2)	.	.	.	yes
O8A	C81A	H812"	149.00	.	.	.	no
O8A	C81A	H811"	110.00	.	.	.	no
C81B	C81A	H811"	93.00	.	.	.	no
O8A	C81A	H811	109.00	.	.	.	no
C81B	C81A	H811'	27.00	.	.	.	no
H811'	C81A	H811"	110.00	.	.	.	no
H811'	C81A	H812"	74.00	.	.	.	no
H811'	C81A	H811	109.00	.	.	.	no
H811"	C81A	H812"	97.00	.	.	.	no
H811"	C81A	H811	109.00	.	.	.	no
C81B	C81A	H812"	53.00	.	.	.	no
C81B	C81A	H811	96.00	.	.	.	no
O8A	C81A	H811'	110.00	.	.	.	no
H812"	C81A	H811	44.00	.	.	.	no
O8B	C81B	H812"	109.00	.	.	.	no
O8B	C81B	H812	110.00	.	.	.	no
C81A	C81B	H812'	91.00	.	.	.	no
C81A	C81B	H812"	25.00	.	.	.	no
C81A	C81B	H811'	54.00	.	.	.	no

H811'	C81B	H812'	37.00	.	.	.	no
H811'	C81B	H812"	73.00	.	.	.	no
H811'	C81B	H812	117.00	.	.	.	no
H812'	C81B	H812"	109.00	.	.	.	no
H812'	C81B	H812	109.00	.	.	.	no
H812"	C81B	H812	110.00	.	.	.	no
C81A	C81B	H812	101.00	.	.	.	no
O8B	C81B	H811'	130.00	.	.	.	no
O8B	C81B	H812'	109.00	.	.	.	no

loop_

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 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag

S2	Fe	S1	C9	78.94 (14)	.	.	.	no
O3	Fe	S1	C9	-104.02 (16)	.	.	.	no
N1	Fe	S1	C9	-13.77 (17)	.	.	.	no
N5	Fe	S1	C9	163.55 (17)	.	.	.	no
S1	Fe	S2	C18	79.39 (16)	.	.	.	no
O1	Fe	S2	C18	-102.02 (17)	.	.	.	no
N1	Fe	S2	C18	164.30 (19)	.	.	.	no
N5	Fe	S2	C18	-13.68 (19)	.	.	.	no
S2	Fe	O1	C6	-122.2 (3)	.	.	.	no
O3	Fe	O1	C6	60.8 (3)	.	.	.	no
N1	Fe	O1	C6	-29.3 (3)	.	.	.	no
N5	Fe	O1	C6	153.2 (3)	.	.	.	no
S1	Fe	O3	C15	-129.6 (3)	.	.	.	no
O1	Fe	O3	C15	52.0 (3)	.	.	.	no
N1	Fe	O3	C15	145.4 (3)	.	.	.	no
N5	Fe	O3	C15	-36.7 (3)	.	.	.	no
S1	Fe	N1	N3	21.2 (3)	.	.	.	no
S1	Fe	N1	C1	-162.2 (3)	.	.	.	no
S2	Fe	N1	N3	-67.0 (3)	.	.	.	no
S2	Fe	N1	C1	109.7 (3)	.	.	.	no
O1	Fe	N1	N3	-161.6 (3)	.	.	.	no
O1	Fe	N1	C1	15.1 (3)	.	.	.	no
O3	Fe	N1	N3	111.1 (3)	.	.	.	no
O3	Fe	N1	C1	-72.2 (3)	.	.	.	no
S1	Fe	N5	N7	-67.0 (3)	.	.	.	no
S1	Fe	N5	C10	113.0 (3)	.	.	.	no
S2	Fe	N5	N7	21.1 (3)	.	.	.	no
S2	Fe	N5	C10	-158.9 (4)	.	.	.	no
O1	Fe	N5	N7	115.7 (3)	.	.	.	no
O1	Fe	N5	C10	-64.3 (4)	.	.	.	no
O3	Fe	N5	N7	-157.2 (3)	.	.	.	no
O3	Fe	N5	C10	22.9 (4)	.	.	.	no
Fe	S1	C9	N3	9.3 (4)	.	.	.	no
Fe	S1	C9	N4	-171.3 (3)	.	.	.	no
Fe	S2	C18	N7	9.5 (4)	.	.	.	no
Fe	S2	C18	N8	-169.7 (4)	.	.	.	no
Fe	O1	C6	C2	26.9 (5)	.	.	.	no
Fe	O1	C6	C5	-153.1 (3)	.	.	.	no
Fe	O3	C15	C11	29.6 (5)	.	.	.	no
Fe	O3	C15	C14	-151.0 (3)	.	.	.	no

Fe	N1	N3	C9	-19.8 (4)	no
C1	N1	N3	C9	163.1 (4)	no
Fe	N1	C1	C2	3.2 (6)	no
N3	N1	C1	C2	-179.9 (4)	no
C5	N2	C4	C3	-2.6 (6)	no
C4	N2	C5	C6	-0.3 (6)	no
C4	N2	C5	C8	177.4 (4)	no
N1	N3	C9	S1	4.1 (5)	no
N1	N3	C9	N4	-175.4 (4)	no
Fe	N5	N7	C18	-19.6 (4)	no
C10	N5	N7	C18	160.4 (4)	no
Fe	N5	C10	C11	-0.1 (6)	no
N7	N5	C10	C11	179.9 (4)	no
C14	N6	C13	C12	0.3 (7)	no
C13	N6	C14	C15	0.1 (6)	no
C13	N6	C14	C17	179.9 (4)	no
N5	N7	C18	S2	3.7 (5)	no
N5	N7	C18	N8	-177.1 (4)	no
N1	C1	C2	C3	167.5 (4)	no
N1	C1	C2	C6	-15.1 (7)	no
C1	C2	C3	C4	179.2 (4)	no
C1	C2	C3	C7	-1.6 (6)	no
C6	C2	C3	C4	1.7 (6)	no
C6	C2	C3	C7	-179.1 (4)	no
C1	C2	C6	O1	-1.8 (7)	no
C1	C2	C6	C5	178.3 (4)	no
C3	C2	C6	O1	175.6 (4)	no
C3	C2	C6	C5	-4.4 (6)	no
C2	C3	C4	N2	1.9 (6)	no
C7	C3	C4	N2	-177.3 (4)	no
C2	C3	C7	O2	-62.8 (5)	no
C4	C3	C7	O2	116.5 (4)	no
N2	C5	C6	O1	-176.2 (4)	no
N2	C5	C6	C2	3.7 (6)	no
C8	C5	C6	O1	6.2 (6)	no
C8	C5	C6	C2	-173.8 (4)	no
N5	C10	C11	C12	162.7 (4)	no
N5	C10	C11	C15	-19.2 (7)	no
C10	C11	C12	C13	177.1 (4)	no
C10	C11	C12	C16	-5.4 (6)	no
C15	C11	C12	C13	-1.1 (6)	no
C15	C11	C12	C16	176.5 (4)	no
C10	C11	C15	O3	2.7 (6)	no
C10	C11	C15	C14	-176.7 (4)	no
C12	C11	C15	O3	-179.2 (4)	no
C12	C11	C15	C14	1.4 (6)	no
C11	C12	C13	N6	0.2 (7)	no
C16	C12	C13	N6	-177.4 (4)	no
C11	C12	C16	O4	-65.1 (5)	no
C13	C12	C16	O4	112.5 (4)	no
N6	C14	C15	O3	179.6 (4)	no
N6	C14	C15	C11	-1.0 (6)	no
C17	C14	C15	O3	-0.2 (6)	no
C17	C14	C15	C11	179.2 (4)	no
O8A	C81A	C81B	O8B	120 (4)	no

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loop_
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_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1

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_geom_contact_site_symmetry_2

_geom_contact_publ_flag

Fe	H61	3.31 (5)	.	.	no
Fe	H27'	3.48 (6)	.	2_676	no
S1	S2	3.1407 (17)	.	.	no
S1	O3	2.965 (3)	.	.	no
S1	N1	2.826 (4)	.	.	no
S1	N3	2.711 (4)	.	.	no
S1	N5	3.029 (4)	.	.	no
S1	N7	3.458 (4)	.	.	no
S1	C18	3.458 (5)	.	.	no
S1	S1	3.6744 (17)	.	2_576	no
S1	N4	3.471 (5)	.	2_576	no
S2	N1	3.024 (4)	.	.	no
S2	N7	2.712 (4)	.	.	no
S2	C9	3.450 (5)	.	.	no
S2	S1	3.1407 (17)	.	.	no
S2	O1	3.086 (3)	.	.	no
S2	N3	3.444 (4)	.	.	no
S2	N5	2.821 (3)	.	.	no
S2	C4	3.639 (5)	.	2_675	no
S1	H61	3.13 (6)	.	.	no
S1	H16	2.99 (4)	.	2_666	no
S1	H26'	2.92 (5)	.	2_576	no
S2	H4	2.89 (5)	.	2_675	no
O1	S2	3.086 (3)	.	.	no
O1	O3	2.669 (5)	.	.	no
O1	N1	2.808 (5)	.	.	no
O1	N5	2.696 (4)	.	.	no
O1	C1	2.946 (5)	.	.	no
O1	C10	3.156 (4)	.	.	no
O1	C11	3.143 (5)	.	.	no
O1	C15	2.935 (5)	.	.	no
O1	N8	3.100 (5)	.	2_676	no
O2	C1	3.060 (5)	.	.	no
O2	C81B	2.71 (2)	.	.	no
O2	C81A	2.73 (7)	.	.	no
O2	N6	2.707 (5)	.	2_665	no
O2	N4	2.918 (6)	.	2_575	no
O3	O6	2.926 (6)	.	.	no
O3	C10	2.932 (5)	.	.	no
O3	N5	2.776 (4)	.	.	no
O3	N1	2.726 (4)	.	.	no
O3	O1	2.669 (5)	.	.	no
O3	C6	3.049 (5)	.	.	no
O3	C2	3.346 (5)	.	.	no
O3	S1	2.965 (3)	.	.	no
O3	C1	3.282 (5)	.	.	no
O4	N8	3.074 (5)	.	2_676	no
O4	C10	3.128 (6)	.	.	no
O4	O5	2.838 (5)	.	1_655	no
O4	O5	2.817 (5)	.	2_666	no
O5	O4	2.838 (5)	.	1_455	no
O5	C16	3.321 (6)	.	2_666	no
O5	O7	2.919 (6)	.	.	no
O5	O6	2.768 (6)	.	.	no
O5	O4	2.817 (5)	.	2_666	no
O6	C81B	2.88 (2)	.	.	no
O6	O3	2.926 (6)	.	.	no
O6	O5	2.768 (6)	.	.	no
O6	O8B	2.856 (11)	.	.	no

O6	C17	3.336 (7)	.	.	no
O6	O8A	2.957 (12)	.	.	no
O6	C81A	2.49 (2)	.	.	no
O7	N2	2.831 (7)	.	2_665	no
O7	C81B	2.52 (2)	.	2_565	no
O7	N3	2.994 (6)	.	1_545	no
O7	C81A	2.80 (5)	.	2_565	no
O7	O8A	2.807 (13)	.	2_565	no
O7	O5	2.919 (6)	.	.	no
O8A	O6	2.957 (12)	.	.	no
O8A	O7	2.807 (13)	.	2_565	no
O8A	N2	3.070 (10)	.	2_665	no
O8B	O6	2.856 (11)	.	.	no
O8B	C1	3.382 (12)	.	2_575	no
O8B	N3	3.128 (9)	.	2_575	no
O8B	N3	2.837 (11)	.	.	no
O8B	C9	3.386 (10)	.	.	no
O1	H27 '	2.33 (5)	.	2_676	no
O1	H8	2.74 (5)	.	.	no
O2	H26	2.08 (6)	.	2_575	no
O2	H1	2.61 (4)	.	.	no
O2	H811 "	1.8300	.	.	no
O2	H812 "	2.7000	.	.	no
O2	H812	1.9600	.	.	no
O3	H61	2.08 (5)	.	.	no
O3	H16 '	2.79 (4)	.	2_666	no
O3	H17 '	2.58 (5)	.	.	no
O3	H17	2.89 (4)	.	.	no
O4	H10	2.77 (4)	.	.	no
O4	H51 '	2.10 (9)	.	2_666	no
O4	H27	2.29 (5)	.	2_676	no
O5	H24	2.08 (10)	.	1_455	no
O5	H71 '	2.10 (5)	.	.	no
O6	H51	1.92 (7)	.	.	no
O6	H812 "	2.2200	.	.	no
O6	H811	1.6200	.	.	no
O6	H82	2.8700	.	.	no
O6	H17	2.63 (4)	.	.	no
O6	H811 '	2.8200	.	.	no
O7	H25	2.02 (12)	.	2_665	no
O7	H812	2.6200	.	2_565	no
O7	H811 '	2.1700	.	2_565	no
O7	H81	2.1700	.	2_565	no
O7	H812 '	1.6800	.	2_565	no
O8A	H25	2.88 (11)	.	2_665	no
O8A	H71	2.23 (8)	.	2_565	no
O8A	H61 '	2.83 (6)	.	.	no
O8A	H71	2.78 (7)	.	.	no
O8B	H1	2.51 (5)	.	2_575	no
O8B	H61 '	2.00 (6)	.	.	no
N1	S2	3.024 (4)	.	.	no
N1	O3	2.726 (4)	.	.	no
N1	C6	2.954 (6)	.	.	no
N1	S1	2.826 (4)	.	.	no
N1	O1	2.808 (5)	.	.	no
N1	C9	2.259 (5)	.	.	no
N2	C1	3.410 (5)	.	2_675	no
N2	O8A	3.070 (10)	.	2_665	no
N2	O7	2.831 (7)	.	2_665	no
N3	O7	2.994 (6)	.	1_565	no
N3	O8B	3.128 (9)	.	2_575	no

N3	O8B	2.837 (11)	.	.	no
N3	S2	3.444 (4)	.	.	no
N3	C81B	3.01 (2)	.	2_575	no
N3	S1	2.711 (4)	.	.	no
N4	S1	3.471 (5)	.	2_576	no
N4	O2	2.918 (6)	.	2_575	no
N4	C18	3.442 (6)	.	2_576	no
N5	S1	3.029 (4)	.	.	no
N5	O3	2.776 (4)	.	.	no
N5	N8	3.145 (6)	.	2_676	no
N5	O1	2.696 (4)	.	.	no
N5	C18	2.244 (5)	.	.	no
N5	C15	2.943 (5)	.	.	no
N5	S2	2.821 (3)	.	.	no
N6	O2	2.707 (5)	.	2_665	no
N7	C18	3.214 (6)	.	2_676	no
N7	S1	3.458 (4)	.	.	no
N7	S2	2.712 (4)	.	.	no
N7	N8	3.299 (6)	.	2_676	no
N8	O4	3.074 (5)	.	2_676	no
N8	O1	3.100 (5)	.	2_676	no
N8	C10	3.170 (6)	.	2_676	no
N8	N5	3.145 (6)	.	2_676	no
N8	N7	3.299 (6)	.	2_676	no
N2	H71	2.82 (8)	.	2_665	no
N3	H812	2.5400	.	2_575	no
N4	H13	2.88 (5)	.	1_465	no
N4	H812	2.9100	.	2_575	no
N5	H27'	2.92 (6)	.	2_676	no
N6	H811"	2.8500	.	2_665	no
N6	H22	1.92 (6)	.	2_665	no
N7	H7	2.71 (5)	.	1_556	no
N7	H26'	2.87 (6)	.	2_576	no
C1	C4	3.507 (6)	.	2_675	no
C1	O2	3.060 (5)	.	.	no
C1	O8B	3.382 (12)	.	2_575	no
C1	N2	3.410 (5)	.	2_675	no
C2	O3	3.346 (5)	.	.	no
C2	C3	3.509 (6)	.	2_675	no
C2	C4	3.577 (6)	.	2_675	no
C3	C6	3.369 (6)	.	2_675	no
C3	C2	3.509 (6)	.	2_675	no
C4	C1	3.507 (6)	.	2_675	no
C4	S2	3.639 (5)	.	2_675	no
C4	C2	3.577 (6)	.	2_675	no
C4	C17	3.458 (7)	.	2_665	no
C6	C7	3.521 (6)	.	2_675	no
C6	C15	3.291 (6)	.	.	no
C6	C3	3.369 (6)	.	2_675	no
C7	C6	3.521 (6)	.	2_675	no
C9	O8B	3.386 (10)	.	.	no
C10	C13	3.331 (6)	.	2_666	no
C10	O4	3.128 (6)	.	.	no
C10	C12	3.386 (6)	.	2_666	no
C10	N8	3.170 (6)	.	2_676	no
C11	O1	3.143 (5)	.	.	no
C11	C11	3.390 (6)	.	2_666	no
C11	C12	3.409 (6)	.	2_666	no
C12	C11	3.409 (6)	.	2_666	no
C12	C10	3.386 (6)	.	2_666	no
C13	C10	3.331 (6)	.	2_666	no

C15	C16	3.512 (6)	.	2_666	no
C15	C6	3.291 (6)	.	.	no
C16	O5	3.321 (6)	.	2_666	no
C16	C15	3.512 (6)	.	2_666	no
C17	C17	3.548 (7)	.	2_665	no
C17	O6	3.336 (7)	.	.	no
C17	C4	3.458 (7)	.	2_665	no
C18	C18	3.282 (6)	.	2_676	no
C18	N4	3.442 (6)	.	2_576	no
C18	N7	3.214 (6)	.	2_676	no
C81A	O7	2.80 (6)	.	2_565	no
C81A	O6	2.49 (2)	.	.	no
C81A	O2	2.73 (7)	.	.	no
C81B	O6	2.88 (2)	.	.	no
C81B	O7	2.52 (2)	.	2_565	no
C81B	O2	2.71 (2)	.	.	no
C81B	N3	3.01 (2)	.	2_575	no
C1	H7'	2.91 (5)	.	.	no
C3	H17"	3.07 (5)	.	2_665	no
C4	H17	3.08 (4)	.	2_665	no
C4	H17"	3.03 (5)	.	2_665	no
C5	H7'	2.90 (5)	.	2_675	no
C6	H7'	2.98 (5)	.	2_675	no
C7	H26	2.79 (6)	.	2_575	no
C7	H27'	3.04 (5)	.	1_554	no
C7	H1	2.54 (5)	.	.	no
C8	H82	2.8600	.	1_655	no
C8	H7'	2.99 (5)	.	2_675	no
C10	H27	2.81 (6)	.	2_676	no
C10	H16'	2.81 (4)	.	.	no
C11	H8	2.95 (6)	.	.	no
C12	H8	2.94 (6)	.	.	no
C13	H22	2.85 (6)	.	2_665	no
C14	H22	2.84 (6)	.	2_665	no
C14	H10	3.10 (4)	.	2_666	no
C15	H61	3.08 (5)	.	.	no
C15	H16'	2.76 (5)	.	2_666	no
C16	H10	2.57 (4)	.	.	no
C16	H51'	2.72 (9)	.	2_666	no
C17	H22	3.05 (6)	.	2_665	no
C17	H17"	3.00 (5)	.	2_665	no
C17	H61	2.88 (6)	.	.	no
C18	H26'	2.83 (5)	.	2_576	no
C81A	H61	2.80 (7)	.	.	no
C81A	H17'	2.99 (8)	.	.	no
C81A	H22	2.74 (8)	.	.	no
C81A	H71	2.59 (10)	.	2_565	no
C81A	H61'	2.03 (7)	.	.	no
C81B	H22	2.97 (6)	.	.	no
C81B	H61'	2.13 (6)	.	.	no
C81B	H71	2.62 (7)	.	2_565	no
H1	O8B	2.51 (5)	.	2_575	no
H1	H7'	2.34 (7)	.	.	no
H1	O2	2.61 (4)	.	.	no
H1	C7	2.54 (5)	.	.	no
H1	H82	2.2100	.	2_575	no
H811'	H61'	2.1700	.	.	no
H811'	H71	2.1300	.	2_565	no
H811'	O7	2.1700	.	2_565	no
H811'	O6	2.8200	.	.	no
H811"	H22	1.7700	.	.	no

H811"	O2	1.8300	.	.	no
H811"	N6	2.8500	.	2_665	no
H812'	H61'	2.5700	.	.	no
H812'	H71'	2.4800	.	2_565	no
H812'	H71	1.7200	.	2_565	no
H812'	H25	2.4700	.	1_455	no
H812'	H81	2.0300	.	.	no
H812'	O7	1.6800	.	2_565	no
H4	S2	2.89(5)	.	2_675	no
H4	H7	2.28(7)	.	.	no
H812"	O2	2.7000	.	.	no
H812"	H61'	1.6400	.	.	no
H812"	H61	2.5000	.	.	no
H812"	O6	2.2200	.	.	no
H7	H27'	2.58(7)	.	1_554	no
H7	N7	2.71(5)	.	1_554	no
H7	H4	2.28(7)	.	.	no
H7'	H27'	2.54(7)	.	1_554	no
H7'	C1	2.91(5)	.	.	no
H7'	H1	2.34(7)	.	.	no
H7'	C6	2.98(5)	.	2_675	no
H7'	H8"	2.43(8)	.	2_675	no
H7'	C8	2.99(5)	.	2_675	no
H7'	C5	2.90(5)	.	2_675	no
H8	O1	2.74(5)	.	.	no
H8	C12	2.94(6)	.	.	no
H8	C11	2.95(6)	.	.	no
H8'	H81	2.5600	.	2_665	no
H8'	H25	2.30(13)	.	.	no
H8"	H7'	2.43(8)	.	2_675	no
H8"	H82	2.3000	.	1_655	no
H10	O4	2.77(4)	.	.	no
H10	H16'	2.16(6)	.	.	no
H10	C14	3.10(4)	.	2_666	no
H10	C16	2.57(4)	.	.	no
H13	N4	2.88(5)	.	1_645	no
H13	H16	2.34(7)	.	.	no
H16	S1	2.99(4)	.	2_666	no
H16	H13	2.34(7)	.	.	no
H16'	H51'	2.54(9)	.	2_666	no
H16'	C15	2.76(5)	.	2_666	no
H16'	H10	2.16(6)	.	.	no
H16'	C10	2.81(4)	.	.	no
H16'	O3	2.79(4)	.	2_666	no
H17	C4	3.08(4)	.	2_665	no
H17	O3	2.89(4)	.	.	no
H17	H61	2.37(7)	.	.	no
H17	O6	2.63(4)	.	.	no
H17'	O3	2.58(5)	.	.	no
H17'	H61	2.56(7)	.	.	no
H17'	C81A	2.99(8)	.	.	no
H17'	H811	2.5200	.	.	no
H17'	H17"	2.52(7)	.	2_665	no
H17"	H17'	2.52(7)	.	2_665	no
H17"	C4	3.03(5)	.	2_665	no
H17"	H22	2.44(8)	.	2_665	no
H17"	C3	3.07(5)	.	2_665	no
H17"	C17	3.00(5)	.	2_665	no
H22	C81B	2.97(6)	.	.	no
H22	C81A	2.74(8)	.	.	no
H22	H26	2.29(8)	.	2_575	no

H22	C13	2.85 (6)	.	2_665	no
H22	H811"	1.7700	.	.	no
H22	C17	3.05 (6)	.	2_665	no
H22	H812	2.2600	.	.	no
H22	C14	2.84 (6)	.	2_665	no
H22	H17"	2.44 (8)	.	2_665	no
H22	N6	1.92 (6)	.	2_665	no
H24	O5	2.08 (10)	.	1_655	no
H24	H51	2.46 (12)	.	1_655	no
H24	H51'	2.47 (13)	.	1_655	no
H24	H51'	2.47 (13)	.	2_666	no
H24	H27	2.48 (11)	.	2_676	no
H25	O7	2.02 (12)	.	2_665	no
H25	H812'	2.4700	.	1_655	no
H25	O8A	2.88 (11)	.	2_665	no
H25	H8'	2.30 (13)	.	.	no
H25	H71	2.03 (14)	.	2_665	no
H26	H22	2.29 (8)	.	2_575	no
H26	C7	2.79 (6)	.	2_575	no
H26	O2	2.08 (6)	.	2_575	no
H26	H812	2.2000	.	2_575	no
H26'	C18	2.83 (5)	.	2_576	no
H26'	S1	2.92 (5)	.	2_576	no
H26'	N7	2.87 (6)	.	2_576	no
H27	O4	2.29 (5)	.	2_676	no
H27	H24	2.48 (11)	.	2_676	no
H27	C10	2.81 (6)	.	2_676	no
H27'	H7'	2.54 (7)	.	1_556	no
H27'	Fe	3.48 (6)	.	2_676	no
H27'	O1	2.33 (5)	.	2_676	no
H27'	H7	2.58 (7)	.	1_556	no
H27'	C7	3.04 (5)	.	1_556	no
H27'	N5	2.92 (6)	.	2_676	no
H51	H61'	2.56 (9)	.	.	no
H51	O6	1.92 (7)	.	.	no
H51	H71'	2.46 (9)	.	.	no
H51	H61	2.51 (9)	.	.	no
H51	H24	2.46 (12)	.	1_455	no
H51'	H71'	2.42 (10)	.	.	no
H51'	H24	2.47 (13)	.	2_666	no
H51'	H24	2.47 (13)	.	1_455	no
H51'	C16	2.72 (8)	.	2_666	no
H51'	H16'	2.54 (9)	.	2_666	no
H51'	O4	2.10 (9)	.	2_666	no
H61	O3	2.08 (5)	.	.	no
H61	C15	3.08 (5)	.	.	no
H61	Fe	3.31 (5)	.	.	no
H61	S1	3.13 (6)	.	.	no
H61	H811	1.8300	.	.	no
H61	H51	2.51 (9)	.	.	no
H61	H812"	2.5000	.	.	no
H61	C17	2.88 (6)	.	.	no
H61	C81A	2.80 (7)	.	.	no
H61	H17	2.37 (7)	.	.	no
H61	H17'	2.56 (7)	.	.	no
H61'	C81A	2.03 (7)	.	.	no
H61'	O8B	2.00 (6)	.	.	no
H61'	H811	1.2300	.	.	no
H61'	C81B	2.13 (6)	.	.	no
H61'	H811'	2.1700	.	.	no
H61'	H812'	2.5700	.	.	no

H61'	H812"	1.6400	.	.	no
H61'	H51	2.56(9)	.	.	no
H61'	H82	2.0800	.	.	no
H61'	O8A	2.83(6)	.	.	no
H71	H81	1.4700	.	2_565	no
H71	O8A	2.23(8)	.	2_565	no
H71	N2	2.82(8)	.	2_665	no
H71	C81A	2.59(10)	.	2_565	no
H71	C81B	2.62(7)	.	2_565	no
H71	H811'	2.1300	.	2_565	no
H71	O8A	2.78(7)	.	.	no
H71	H81	2.5300	.	.	no
H71	H25	2.03(14)	.	2_665	no
H71	H812'	1.7200	.	2_565	no
H71'	H51'	2.42(10)	.	.	no
H71'	H51	2.46(9)	.	.	no
H71'	O5	2.10(5)	.	.	no
H71'	H812'	2.4800	.	2_565	no
H71'	H81	2.4800	.	2_565	no
H81	H71'	2.4800	.	2_565	no
H81	H812'	2.0300	.	.	no
H81	H71	2.5300	.	.	no
H81	O7	2.1700	.	2_565	no
H81	H8'	2.5600	.	2_665	no
H81	H71	1.4700	.	2_565	no
H82	O6	2.8700	.	.	no
H82	C8	2.8600	.	1_455	no
H82	H8"	2.3000	.	1_455	no
H82	H61'	2.0800	.	.	no
H82	H1	2.2100	.	2_575	no
H811	O6	1.6200	.	.	no
H811	H17'	2.5200	.	.	no
H811	H61	1.8300	.	.	no
H811	H61'	1.2300	.	.	no
H812	O2	1.9600	.	.	no
H812	H22	2.2600	.	.	no
H812	O7	2.6200	.	2_565	no
H812	N3	2.5400	.	2_575	no
H812	N4	2.9100	.	2_575	no
H812	H26	2.2000	.	2_575	no

loop_

_geom_hbond_atom_site_label_D

_geom_hbond_atom_site_label_H

_geom_hbond_atom_site_label_A

_geom_hbond_distance_DH

_geom_hbond_distance_HA

_geom_hbond_distance_DA

_geom_hbond_angle_DHA

_geom_hbond_site_symmetry_A

_geom_hbond_publ_flag

#

#D H A D - H H...A D...A D - H...A symm(A)

#

O2	H22	N6	0.79(6)	1.92(6)	2.707(5)	171(7)	2_665	yes
O4	H24	O5	0.84(10)	2.08(10)	2.838(5)	151(9)	1_655	yes
N2	H25	O7	0.82(12)	2.02(12)	2.831(7)	168(12)	2_665	yes
N4	H26	O2	0.86(6)	2.08(6)	2.918(6)	166(6)	2_575	yes
N8	H27	O4	0.80(5)	2.29(5)	3.074(5)	167(5)	2_676	yes
N8	H27'	O1	0.88(5)	2.33(5)	3.100(5)	146(4)	2_676	yes
O5	H51	O6	0.86(7)	1.92(7)	2.768(6)	171(6)	.	yes

O5	H51'	O4	0.86(9)	2.10(9)	2.817(5)	141(8)	2_666	yes
O6	H61	O3	0.85(5)	2.08(5)	2.926(6)	172(6)	.	yes
O6	H61'	O8B	0.86(5)	2.00(6)	2.856(11)	175(6)	.	yes
O7	H71	O8A	0.91(4)	2.23(8)	2.807(13)	121(7)	2_565	yes
O7	H71'	O5	0.87(4)	2.10(5)	2.919(6)	158(5)	.	yes
O8A	H81	O7	0.8400	2.1700	2.807(13)	133.00	2_565	yes
C1	H1	O8B	0.94(5)	2.51(5)	3.382(12)	154(4)	2_575	yes
C81A	H811'	O7	0.9800	2.1700	2.80(6)	121.00	2_565	yes
C81A	H811"	O2	0.9800	1.8300	2.73(7)	152.00	.	yes
C81B	H812'	O7	0.9800	1.6800	2.52(2)	141.00	2_565	yes
C81A	H812"	O6	0.5200	2.2200	2.49(2)	115.00	.	yes
C81A	H811	O6	0.9800	1.6200	2.49(2)	145.00	.	yes
C81B	H812	O2	0.9800	1.9600	2.71(2)	132.00	.	yes
C81B	H812	N3	0.9800	2.5400	3.01(2)	110.00	2_575	yes

Loop Mechanism for Extra Tables(s)

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#_publ_manuscript_incl_extra_item
#'_geom_extra_tableA_col_1'
#'_geom_extra_tableA_col_2'
#'_geom_extra_tableA_col_3'
#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
#'_geom_extra_tableB_col_3'
#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'
```

```
#
#loop_
#_geom_extra_tableA_col_1
#_geom_extra_tableA_col_2
#_geom_extra_tableA_col_3
# ? ? ?
```

```
#
#loop_
#_geom_extra_tableB_col_1
#_geom_extra_tableB_col_2
#_geom_extra_tableB_col_3
# ? ? ?
```

```
#
#_geom_table_footnote_A
#;
# ?
#;
```

```
#
#_geom_table_footnote_B
#;
# ?
#;
```

```
#  
#_geom_table_footnote_A  
#;  
# ?  
#;
```

```
#  
#_geom_table_footnote_B  
#;  
# ?  
#;
```

```
#===END of Crystallographic Information File
```